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Oscillator strengths of the allowed np-n'd and nd-n'f transitions in the helium isoelectronic sequence

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Oscillator strengths for allowed $np-n'd$ and $nd-n'f$ transitions for some members of the helium isoelectronic sequence have been calculated by utilizing dipole length, velocity and acceleration forms of the transition matrix element with coupled H.F. wavefunctions. Comparisons have been made with the available experimental values and also with other theoretical values and their implications are discussed.

1. INTRODUCTION

Determination of accurate values of the oscillator strengths (f values) for electric dipole transitions has been the subject of considerable interest in atomic spectroscopy. The importance of these fundamental atomic data has been enhanced in view of the advances made in laboratory plasma physics and sattelite astronomy. Accurate values of the oscillator strengths now help to acertain the most abundant element in the spectrum of solar corona. These data are also being used to establish models for stellar atmosphere where highly excited states of highly positive ions are predominant. Studies on the soft X-ray spectra of solar flares indicate the presence of some emission lines from the members of the Helium isoelectronic series extending as far as CaXIX (Meekings *et al* 1968) in one case and as far as FeXXV in another (Neupert *et al* 1967). Studies on ionization-equilibrium suggest that at the solar corona temperature the two-electron ions of lighter element may be a dominant species (Cox *et al* 1969). In this paper we present the values of the oscillator strength for $1snp-isn'd$ and $1snd-1Sn'f$ spectral transitions for some member of the Helium isoelectronic series using coupled HF wave functions as described in section 2. In view of much uncertainty in the theoretical values systematic calculations of oscillator strength with variety of wave functions seem necessary.

2. WAVE FUNCTIONS AND CALCULATION OF OSCILLATOR STRENGTHS

The dynamic polarizability of an atom under the influence of a perturbing electromagnetic field of varying frequency exhibit singularities. These singularities are related to one-electron excitations. Approximate wave functions for the excited states may be obtained from a study of the perturbed wave function in the neighbourhood of the singularities, (Mukherjee *et al* 1969). The wave func-

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tion represents a situation where one of the electron is in the excited state while the other remain in the initial orbital. The interelectronic interactions are different in the ground state and excited state. Incorporating the required relaxation effect, coupled H.F. wave functions for the different excited state configuration of the members of the Helium isoelectronic sequence were obtained through a self consistent variation perturbation procedure (Mukherjee *et al* 1970, 1971; Maitra *et al* 1970). The wave functions without the relaxation effect obtained in polarizability calculation were used as the starting wave function. The final wave functions are tabulated in the above metioned references. These wave functions yielded very satisfactory results for the dipole and quadrupole properties for the two and three-electron atoms and ions (Sengupta 1975, Datta *et al* 1976). The wave functions were taken to be of the form $\sum_i C_i r^{n_i} e^{-\zeta_i r} y_l^m$ for respective states under consideration. The parameters C_i, n_i and ξ_i are listed in the above mentioned references. The result revealed some interesting dependence of the values of oscillator strengths on the nuclear charge Z.

Standard expressions for the dipole length ((f_L), velocity (f_V) and acceleration (f_A) forms of the oscillator strength have been used. They are

$$f_L = 2(E_m - E_0) \left| < \psi_m | z_1 + z_2 | \psi_0 > \right|^2 \quad \ldots (1)$$

$$f_V = \frac{2}{(E_m - E_0)} \left| < \psi_m \left| \frac{\partial}{\partial z_1} + \frac{\partial}{\partial z_2} \right| \psi_0 > \right|^2 \quad \ldots (2)$$

$$f_A = \frac{2}{(E_m - E_0)^3} \left| Z < \psi_m \left| \frac{z_1}{r_1^3} + \frac{z_2}{r_2^3} \right| \psi_0 > \right|^2 \quad \ldots (3)$$

respectively. Agreement among these three values, though not mandatory, has often been used to assess the accuracy of the calculated values of oscillator strengths.

In cases where the emission of a spectral line occurs through a single transition the oscillator strength f for the transition in question is related to the radiative decay rates A' by (Griem 1964),

$$f = \frac{\lambda^2}{8\pi^2 r_0 c} \cdot \frac{2L'+1}{2L+1} A' \quad \ldots (4)$$

where L' and L are the orbital angular momentum quantum number of upper and lower levels respectively, r_0 is the clasical electron radius c and λ are the velocity of light and wave length of the spectral line respectively. Radiative decay rates of the excited states of Helium atom have been found out by Heron *et al* (1956) and Kindlmann *et al* (1973). Values of the oscillator strengths derived from the decay rates using formula (4) have been referred in appropriate cases along with the computed theoretical values in section III.

3. Results

Values of f_L and f_V for the different spectral transitions in Helium and two-electron positive ions have been given in Table 1. Values of the f_A have been omitted because of poor agreement with f_L and f_V. The discrepancy between f_A and f_L or f_V is logical to expect. While f_A is proportional to the nuclear charge Z the electron taking part in the transition effectively moves in the coulomb field of $Z-1$. We have compared our values with other theoretical values. These include the calculations of Cohen *et al* (1972), Chong (1968), Green and Kolchin (1966), Brown (1969). Their values for the relevant quantities are also cited in table 1 for systematic comparison. For a given spectral transition our values are higher than all other theoretical values. The agreement with experimental values (where it is available) is satisfactory. There is no marked dependence of the values of the oscillator strengths on the nuclear charge Z. Closeness of the values of f_L and f_V indicates the accuracy of the values presented, as well as of the wave functions used. It also suggests that the effect of nonlocal exchange potential on the values of the oscillator strengths becomes increasingly less important while one deals with higher excitation of highly positive ions. For, as shown by Starace (1971), f_L and f_V for an electric dipole transition between states α and β differ by the matrix element of the commutator of the nonlocal exchange potential with the coordinates.

In view of the differences between the values of oscillator strengths computed by different authors it seems necessary that the values of the oscillator strengths should be subjected to accuracy test of Anderson and Weinhold (1974). Also proper assessment should be made of the possible cancellation error which may crop up as the number of nodes in the wave functions increases. Only after these investigations consistent value of the oscillator strengths for transitions involving higher state of excitations can be predicted, and actual dependence of these values on the nuclear charge Z can be studied.

Table 1 : Values of oscillator strengths for some electric dipole transitions in Helium and other members of the isoelectronic series.

Transition		Present		Cohen & McEachran (1972)	Green & Kolchin (1966)		Chong D.P. (1968)	Brown R.T. (1969)	
		f_L	f_V		f_L	f_V		f_L	f_V
2^1P–3^1D	He	·8886	·8486	·724	·7106	·7095	·8712		
	Li^+	·8686	·8645	·723			·8686		
	Be^{++}	·8598	·8622	·718			·8627		
	B^{+++}	·8550	·8578	·714			·8580		
2^1P–4^1D	He	·1513	·1419	·120	·1205	·1202			
	Li^+	·1464	·1441	·121					
	Be^{++}	·1453	·1449	·121					
	B^{+++}	·1448	·1452	·121					

Transation		Present		Cohen & McEachran (1972)	Green & Kolchin (1966)		Chong D,P, (1968)	Brown R,T, (1969)	
		f_L	f_V		f_L	f_V		f_L	f_V
3^1P–4^1D	He	·8664	·7485	·671	·6490	·6486			
	Li^+	·8048	·7875	·665					
	Be^{++}	·7859	·7851	·648					
	B^{+++}	·7763	·7772	·648					
2^3P–3^3D*	He	·7641	·7318	·625	·6105	·6269	·7525		
	Li^+	·7629	·7473	·631			·7549		
	Be^{++}	·7766	·7625	·644			·7683		
	B^{+++}	·7875	·7743	·652			·7792		
2^3P–4^3D	He	·1534	·1448	·123	·1232	·1275			
	Li^+	·1502	·1466	·123					
	Be^{++}	·1492	·1469	·123					
	B^{+++}	·1493	·1469	·123					
3^3P–4^3D	He	·5758	·5935	·500	·4766	·4790			
	Li^+	·6023	·6093	·508					
	Be^{++}	·6527	·6352	·532					
	B^{+++}	·6558	·6527	·546					
3^1D–4^1F	He	1·312	1·304				1·3088		
	Li^+	1·312	1·306				1·3093	1·005	1·015
	Be^{++}	1·309	1·309				1·3093	1·011	1·015
	B^{+++}	1·309	1·309				1·3093	1·014	1·016
4^1D–5^1F	He	1·152	1·142						
	Li^+	1·149	1·144						
	Be^{++}	1·146	1·146						
	B^{+++}	1·146	1·146						
3^3D–4^3F	He	1·310	1·304				1·3072		
	Li^+	1·308	1·304				1·3063	1·005	1·014
	Be^{++}	1·306	1·306				1·3061	1·008	1·013
	B^{+++}	1·306	1·306				1·3062	1·013	1·016
3^3D–5^3F	He	·2020	·2012						
	Li^+	·2021	·2013					·1603	·1579
	Be^{++}	·2019	·2017					·1604	·1574
	B^{+++}	·2019	·2016					·1588	·1569
3^3D–6^3F	He	·0694	·0694						
	Li^+	·0694	·0694					·0550	·0546
	Be^{++}	·0693	·0695					·0542	·0542
	B^{+++}	·0694	·0694					·0539	·0540
4^3D–5^3F	He	1·147	1·139						
	Li^+	1·143	1·137						
	Be^{++}	1·140	1·140						
	B^{+++}	1·140	1·140						
4^3D–6^3F	Li^+	·2389	·2392						
	Be^{++}	·2383	·2393						
	B^{+++}	·2386	·2393						

* For helium value of the experimental oscillator strength corresponding $2'P$–$3'D$ transition is 0·69 by Kidlmann & Bennett (1963), The experimental value corresponding 2^3P–3^3D transition are 0·86 by Heran *et al* (1956) and 0·60 by Kindlmann & Bennett,

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